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Computation of Superconductivity in Thin Films*

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This paper presents a method for computing the physical states in superconducting thin films under the influence of a parallel uniform external magnetic field. The governing equations are the Ginzburg–Landau equations which in general possess multiple solutions and the physical states are those which minimize the total energy. In our approach the energy functional is used to generate a gradient flow and the physical states are obtained in the large time limit. The numerical results completely verify the Meissner effect and the fine structure of the solutions exhibits the occurrence of a symmetric nucleation of superconductivity at intermediate fields. © 1990 Academic Press, Inc.

1. INTRODUCTION

Slightly below the transition temperatures, the behaviour of superconducting materials is governed by the Ginzburg–Landau (GL) differential equations [11]. Although these equations were originally introduced phenomenologically, Gorkov [12] was able to derive them theoretically from his formulation of the Bardeen–Cooper–Schrieffer (BCS) theory where the microscopic structure of a superconductor is replaced by a complex scalar field ϕ which is an order parameter representing the density of superconducting electron pairs and interacting with the excited electromagnetic vector potential **A**. It is more often the GL equations, rather than the BCS theory itself, which have led to technological advances, since they allow practical calculations for various samples. However, on the other hand, except for some extreme cases, the exact solutions of the GL equations are difficult

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to obtain due to the complexity of the system and, in general, suitable approximation methods must be resorted to. In particular, perturbative analysis has shown the destruction of superconductivity in thin films by a magnetic field exceeding a critical external field strength which increases with decreasing thickness of the films [11] and that there exists a third critical field in type II superconductivity, so that, at which, a thin superconducting layer appears on the surface of the film [19]; a shooting method has been employed to find the properties of a class of solutions to the thin film GL elquations [16]; a direct variational method has been used to study the interactions of superconducting vortices in the absence of an external field [15, 18]; and, more recently, the Monte Carlo simulation has widely been applied to the lattice versions of the models in two, three, and four dimensions [6, 7, 13, 14]. All of these are meant to compute the stationary or minimization points of the total energy $E(\phi, \mathbf{A})$.

In this paper, we take a new approach to the above problem. Roughly speaking, we will find the stationary points of $E(\phi, \mathbf{A})$ in the $t \to \infty$ limit of the gradient (or heat) flow $(\phi(t), \mathbf{A}(t))$ generated by the equation $(\phi_t, \mathbf{A}_t) = -\delta E(\phi, \mathbf{A})$, where δ denotes the Fréchet differentiation. Methods of this nature have extensively been used earlier, for example, in the study of the existence of harmonic maps [9, 10]. The purpose of the present paper is to focus exclusively on computing the solutions of the one-dimensional thin film GL equations. It is hoped that our method here may still be explored further to apply to the models in higher dimensions.

We will consider a superconducting film of thickness $2l$ in a parallel (or tangential) constant magnetic field H. In normalized units and reduced variables, the GL equations are [5, 17]:

$$\begin{aligned} &\phi''(x) = \lambda\phi(\phi^2 - 1) + \lambda H^2 A^2 \phi, \\ &A''(x) = \phi^2 A, \qquad -l < x < l; \\ &\phi'(\pm l) = 0, \qquad A'(\pm l) = 1, \end{aligned} \tag{1.1}$$

where, now, ϕ and HA are real scalar fieds representing the order parameter and the electromagnetic potential respectively, $\lambda > 0$ is a dimensionless coupling constant so that $\lambda < \frac{1}{2}$ or $> \frac{1}{2}$ characterizes type I or II superconductors, and the excited magnetic field in the film is given by $B(x) = HA'(x)$. Equations (1.1) are the Euler–Lagrange equations of the total energy (cf. [5])

$$E(\phi, A) = \frac{1}{2}\int_{-l}^{l} dx \left\{ (\phi')^2 + \lambda H^2([A'-1]^2 + A^2\phi^2) + \frac{\lambda}{2}(\phi^2 - 1)^2 \right\}.$$

In general, Eqs. (1.1) may have multiple solutions at different energy levels and the real physical states are those with the least energy value.

If $H = 0$, the only energy minimizers are

$$\phi(x) = \pm 1, \qquad A(x) = \sinh x / \cosh l. \tag{1.2}$$

Our purpose is to compute the energy minimizers at an arbitrary value $H = H_0 \neq 0$. The method is as follows.

Define a time-dependent external field $H(t) \in C[0, \infty)$ connecting the values $H = 0$ and $H = H_0$, i.e., $H(0) = 0$ and $H(t) \equiv H_0$ for $t \geqslant$ some $t_0 > 0$. Insert $H = H(t)$ into the energy $E(\phi, A)$ and switch on the time-dependence of (ϕ, A) according to the convention as mentioned before:

$$(\phi_t, A_t) = -\delta E(\phi, A). \tag{1.3}$$

The equation (1.3) leads to an initial value problem

$$\begin{aligned}
&\phi_t = \phi_{xx} - \lambda\phi(\phi^2 - 1) - \lambda H^2(t)\, A^2\phi, \\
&A_t = A_{xx} - \phi^2 A, \qquad -l < x < l, \qquad t > 0; \\
&\phi_x(\pm l, t) = 0, \qquad A_x(\pm l, t) = 1, \qquad t > 0, \\
&\phi = \phi_0(x), \qquad A = A_0(x), \qquad -l < x < l, \qquad t = 0.
\end{aligned} \tag{1.4}$$

If the initial data (ϕ_0, A_0) are chosen to be physical, namely, (ϕ_0, A_0) satisfies (1.2), then (1.3) or (1.4) determines the time-evolution of the field configurations in a superconducting film (cf., e.g., [2]). It is not hard to prove that [20], as $t \to \infty$, the solutions of (1.4) tend to those of (1.1) which should be the desired least energy solutions at $H = H_0$ by the consistency of the time-evolution equation (1.3) and the least action principle, although a mathematically rigorous justification has not been worked out yet.

In this paper we will integrate Eqs. (1.4) numerically by the backward (implicit) finite difference scheme. Analysis shows that the convergence of the semi-discretized equations is of the second order and that of the backward difference scheme the first order in time and second order in space. A series of numerical results are presented. These results indicate that at small or large external fields, the Meissner effect is complete, that is, the superconducting films behave either like diamagnetic bulk materials or like normal conductors; at intermediate external fields, there is a symmetric nucleation of superconductivity in the middle of the films. For large values of $\lambda > 0$, completely superconducting and normal regions co-exist and, as $\lambda \to \infty$, the superconducting core can be squeezed into an arbitrarily narrow region which implies that a nonlinear desingularization phenomenon [4] occurs in a finite one-dimensional sample in analogy with that in two dimensions [1, 3]. This work shows that the gradient flow method may provide us a very efficient and powerful computational tool in calculating the thin film superconductivity and Eq. (1.3) can indeed yield a correct description of the time-development of the physical solutions of the problem.

2. The Finite Difference Scheme

In order to have a suitable function space setting, we introduce a translation

$$\mathscr{A} = A - x, \qquad \mathscr{A}_0 = A_0 - x.$$

Now Eqs. (1.4) become

$$\begin{aligned} &\phi_t = \phi_{xx} - \lambda\phi(\phi^2 - 1) - \lambda H^2(t)(\mathscr{A} + x)^2 \phi, \\ &\mathscr{A}_t = \mathscr{A}_{xx} - \phi^2(\mathscr{A} + x), \qquad -l < x < l, \qquad t > 0; \\ &\phi_x(\pm l, t) = \mathscr{A}_x(\pm l, t) = 0, \qquad t > 0, \\ &\phi = \phi_0, \qquad \mathscr{A} = \mathscr{A}_0, \qquad -l < x < l, \qquad t = 0. \end{aligned} \tag{2.1}$$

In what follows, we shall use the notation $D^k = \partial^k/\partial x^k$, $H^k(-l, l) = W^{k,2}(-l, l)$, and denote the norms of $H^k(-l, l)$ and $C^k[-l, l]$ by $\| \ \|_k$ and $| \ |_k$ $(k = 0, 1, 2, ...)$, respectively. It has been shown in [20] that, for any $\phi_0, \mathscr{A}_0 \in H^1(-l, l)$ and continuous bounded function $H(t)$ on $[0, \infty)$, Eqs. (2.1) have a unique global classical solution.

Let us first discretize the spatial interval $(-l, l)$ by M equidistant gridpoints

$$x_i = l(2i - M - 1)/M, \qquad i = 1, ..., M$$

with spacing $h = 2l/M$.

For a sufficiently smooth function $w(x)$ on $[-l, l]$ with the boundary condition $Dw(\pm l) = 0$, the central difference scheme leads to the following standard second-order approximation

$$\sup_{1 \leqslant i \leqslant M} |D^2 w(x_i) - (-S\mathbf{w})_i| \leqslant Ch^2 |D^4 w|_0, \tag{2.2}$$

where

$$S = \frac{1}{h^2} \begin{pmatrix} 1 & -1 & 0 & \cdots & \cdots & \cdots & 0 \\ -1 & 2 & -1 & \cdots & \cdots & \cdots & 0 \\ 0 & -1 & 2 & -1 & \cdots & \cdots & 0 \\ 0 & \cdots & \cdots & \cdots & \cdots & \cdots & 0 \\ 0 & \cdots & \cdots & -1 & 2 & -1 & 0 \\ 0 & \cdots & \cdots & \cdots & -1 & 2 & -1 \\ 0 & \cdots & \cdots & \cdots & 0 & -1 & 1 \end{pmatrix}$$

is an $M \times M$ matrix, $\mathbf{w} = (w(x_1), ..., w(x_M))^{\perp}$, and $C > 0$ is a generic constant.

With the notation $\boldsymbol{\psi} = (\psi_1, ..., \psi_M)^{\perp}$, $\boldsymbol{\alpha} = (\alpha_1, ..., \alpha_M)^{\perp}$, $\boldsymbol{\psi}_0 = (\phi_0(x_1), ..., \phi_0(x_M))^{\perp}$, and $\boldsymbol{\alpha}_0 = (\mathscr{A}_0(x_1), ..., \mathscr{A}_0(x_M))^{\perp}$, we may discretize (2.1) into a system of ordinary differential equations in the form

$$\frac{d}{dt}\boldsymbol{\psi} = -S\boldsymbol{\psi} - P_{\psi,\alpha}\boldsymbol{\psi}, \tag{2.3a}$$

$$\frac{d}{dt}\boldsymbol{\alpha} = -S\boldsymbol{\alpha} - Q_{\psi}\boldsymbol{\alpha} - \mathbf{R}_{\psi}, \qquad t>0; \tag{2.3b}$$

$$\boldsymbol{\psi} = \boldsymbol{\psi}_0, \qquad \boldsymbol{\alpha} = \boldsymbol{\alpha}_0, \qquad t=0, \tag{2.3c}$$

where

$$P_{\psi,\alpha} = \lambda \operatorname{diag}\{(\psi_1^2 - 1) + H^2(t)(\alpha_1 + x_1)^2, ..., (\psi_N^2 - 1) + H^2(t)(\alpha_M + x_M)^2\},$$
$$Q_{\psi} = \operatorname{diag}\{\psi_1^2, ..., \psi_M^2\}$$

are diagonal matrices and $\mathbf{R}_{\psi} = (\psi_1^2 x_1, ..., \psi_M^2 x_M)^{\perp}$. The system (2.3) can then be integrated numerically by standard methods.

Our convergence result for the above semi-discretized problem is stated as follows.

THEOREM 2.1. *Suppose $\phi_0, \mathscr{A}_0 \in H^5(-l, l)$ and $(\phi, \mathscr{A})(x, t)$ and $(\boldsymbol{\psi}, \boldsymbol{\alpha})(t)$ are the unique global solutions of Eqs.* (2.1) *and* (2.3), *respectively. Then there exist constants $\delta, \varepsilon > 0$ depending only on $l, \lambda, \|\phi_0\|_5, \|\mathscr{A}_0\|_5$, and $\sup_{t\geq 0}|H(t)|$ such that for any $T>0$, we have the pointwise error estimate*

$$\sup_{1\leq i\leq M, 0\leq t\leq T} \max\{|\phi(x_i, t) - \psi_i(t)|, |\mathscr{A}(x_i, t) - \alpha_i(t)|\} \leq \delta h^2 T e^{\varepsilon T}. \tag{2.4}$$

The inequality (2.4) will be established in Section 3. In the rest part of this section, we only show that the initial value problem (2.3) has a (unique) global solution for any $M>0$.

LEMMA 2.2. *Set $K = \max\{1, |\phi_0|_0\}$ and $K' = \max\{l, |\mathscr{A}_0|_0\}$. For a (local) solution $(\boldsymbol{\psi}, \boldsymbol{\alpha})(t)$ of Eqs.* (2.3), *there hold the following bounds*

$$\sup_{t\geq 0} \max_i\{|\psi_i(t)|\} \leq K, \qquad \sup_{t\geq 0} \max_i\{|\alpha_i(t)|\} \leq K'.$$

Proof. Assume there is a $T>0$ such that $\max_i |\psi_i(T)| > K$. Choose $i_0: 1\leq i_0 \leq M$ and $t_0 \in (0, T]$ to achieve

$$\pm\psi_{i_0}(t_0) = \sup_{0\leq t\leq T} \max_i\{|\psi_i(t)|\}.$$

Suppose first $\psi_{i_0}(t_0) > 0$. Letting $i = i_0$ and $t = t_0$ in (2.3a), we have $-(S\boldsymbol{\psi})_{i_0} \leq 0$ and $d\psi_{i_0}/dt \geq 0$. So $(P_{\psi,\alpha}\boldsymbol{\psi}(t_0))_{i_0} \leq 0$. This is false. Similarly one verifies $\psi_{i_0}(t_0) \nless 0$. This contradiction implies the validity of the bound for $|\psi_i(t)|$.

Let us now prove the bound for $|\alpha_i(t)|$. In fact, from (2.3b), we have

$$\frac{d}{dt}\beta_i^+ \geqslant -(S\boldsymbol{\beta}^+)_i - \psi_i^2\beta_i^+,$$

where $\beta_i^\pm = \alpha_i \pm K'$ and $\boldsymbol{\beta}^\pm = (\beta_1^\pm, ..., \beta_M^\pm)^\perp$.

Obviously, $\beta_i^+ \geqslant 0$ at $t=0$. We claim: $\beta_i^+ \geqslant 0$, $i = 1, ..., M$.

Define $\gamma_i = \beta_i^+ e^{\varepsilon t}$, $\varepsilon > 0$. Then $\boldsymbol{\gamma}$ satisfies

$$\frac{d}{dt}\gamma_i \geqslant -(S\boldsymbol{\gamma})_i - (\psi_i^2 + \varepsilon)\gamma_i, \qquad t \geqslant 0. \tag{2.5}$$

It can be seen that $\gamma_i(t) \geqslant 0$, $i = 1, ..., M$, $t \geqslant 0$. Otherwise, suppose there is some $T > 0$ which makes $\min_{1 \leqslant i \leqslant M}\{\gamma_i(T)\} < 0$. Therefore we can choose i_0: $1 \leqslant i_0 \leqslant M$ and $t_0 \in (0, T]$ such that

$$\gamma_{i_0}(t_0) = \min_{0 \leqslant t \leqslant T} \min_{1 \leqslant i \leqslant M} \{\gamma_i(t)\}.$$

It is easily verified that, at $t = t_0$, $-(S\boldsymbol{\gamma})_{i_0} \geqslant 0$ and $d\gamma_{i_0}/dt \leqslant 0$, which yields $\gamma_{i_0}(t_0) \geqslant 0$, since γ_{i_0} satisfies (2.5) and $\varepsilon > 0$. This is a contradiction. Thus the conclusion $\beta_i^+ \geqslant 0$, $i = 1, ..., M$ follows. Similarly, one establishes $\beta_i^- \leqslant 0$, $i = 1, ..., M$.

The lemma is proved.

In particular, the global solvabilty of Eqs. (2.3) follows.

3. Proof of Convergence

In this section we obtain the error control (2.4).

In $\mathbb{R}^M$, define the integral inner product and the associated norm by

$$(\mathbf{u}, \mathbf{v})_{(h)} = h\sum_{i=1}^{M} u_i v_i, \qquad \|\mathbf{u}\|_{(h)}^2 = (\mathbf{u}, \mathbf{u})_{(h)}, \qquad \mathbf{u}, \mathbf{v} \in \mathbb{R}^M.$$

Let $\mathbf{u} \in \mathbb{R}^M$. There holds

$$(\mathbf{u}, S\mathbf{u})_{(h)} = h^{-1}\sum_{i=1}^{M-1} (u_i - u_{i+1})^2. \tag{3.1}$$

For given $\mathbf{u} \in \mathbb{R}^M$, choose i_0: $1 \leqslant i_0 \leqslant M$ be such that

$$u_{i_0}^2 = \min\{u_1^2, ..., u_M^2\}.$$

Then, by virtue of (3.1), we have

$$u_i^2 \leqslant u_{i_0}^2 + \left(\sum_{j=1}^{M-1} (u_j + u_{j+1})^2 h \right)^{1/2} \left(\sum_{j=1}^{M-1} (u_j - u_{j+1})^2 h^{-1} \right)^{1/2}$$
$$\leqslant \|\mathbf{u}\|_{(h)}^2 / 2l + 2 \|\mathbf{u}\|_{(h)} (\mathbf{u}, S\mathbf{u})_{(h)}^{1/2}. \tag{3.2}$$

This simple inequality will be used in establishing the pointwise error estimate (2.4).

LEMMA 3.1. *Suppose* $\phi_0, \mathscr{A}_0 \in H^k(-l, l)$ $(k \geqslant 1)$ *and* $(\phi, \mathscr{A})(t)$ *is the unique classical solution of Eqs.* (2.1). *There exists a constant* C_1 *depending only on* $l, \lambda, \sup_t |H(t)|, \|\phi_0\|_k$, *and* $\|\mathscr{A}_0\|_k$ *such that*

$$\sup_{t \geqslant 0} \max\{ \|\phi(t)\|_k, \|\mathscr{A}(t)\|_k \} \leqslant C_1.$$

Proof. The case $k = 1$ has been proved in [20]. The general case is easily verified by induction.

Under the condition of Theorem 2.1, we put

$$\boldsymbol{\phi}(t) = (\phi(x_1, t), ..., \phi(x_M, t))^{\perp}, \qquad \boldsymbol{\mathscr{A}}(t) = (\mathscr{A}(x_1, t), ..., \mathscr{A}(x_M, t))^{\perp}.$$

Then, by virtue of (2.2), we can rewrite Eqs. (2.1) in the form

$$\begin{aligned} &\frac{d}{dt}\boldsymbol{\phi} = -S\boldsymbol{\phi} - P_{\phi,\mathscr{A}}\boldsymbol{\phi} + \boldsymbol{\eta}_1, \\ &\frac{d}{dt}\boldsymbol{\mathscr{A}} = -S\boldsymbol{\mathscr{A}} - Q_\phi \boldsymbol{\mathscr{A}} - \mathbf{R}_\phi + \boldsymbol{\eta}_2, \qquad t > 0; \\ &\boldsymbol{\phi} = \boldsymbol{\psi}_0, \qquad \boldsymbol{\mathscr{A}} = \boldsymbol{\alpha}_0, \qquad t = 0, \end{aligned} \tag{3.3}$$

where $P_{\phi,\mathscr{A}}$, Q_ϕ, and $\mathbf{R}_\phi$ are as defined in Section 2 and $\boldsymbol{\eta}_1(t)$, $\boldsymbol{\eta}_2(t)$ satisfy

$$\|\boldsymbol{\eta}_1(t)\|_{(h)}, \qquad \|\boldsymbol{\eta}_2(t)\|_{(h)} \leqslant Ch^2 \tag{3.4}$$

with $C > 0$ depending only on $l, \lambda, \|\phi_0\|_5$, and $\|\mathscr{A}_0\|_5$ as can be seen from Lemma 3.1.

From Eqs. (2.3) and (3.3) one obtains the governing equations for the errors $\boldsymbol{\xi} = \boldsymbol{\phi} - \boldsymbol{\psi}$ and $\boldsymbol{\zeta} = \boldsymbol{\mathscr{A}} - \boldsymbol{\alpha}$ as follows:

$$\begin{aligned} &\frac{d}{dt}\boldsymbol{\xi} = -S\boldsymbol{\xi} - (P_{\phi,\mathscr{A}}\boldsymbol{\phi} - P_{\psi,\alpha}\boldsymbol{\psi}) + \boldsymbol{\eta}_1, \\ &\frac{d}{dt}\boldsymbol{\zeta} = -S\boldsymbol{\zeta} - (Q_\phi \boldsymbol{\mathscr{A}} - Q_\psi \boldsymbol{\alpha}) - (\mathbf{R}_\phi - \mathbf{R}_\psi) + \boldsymbol{\eta}_2, \qquad t > 0; \\ &\boldsymbol{\xi} = 0, \qquad \boldsymbol{\zeta} = 0, \qquad t = 0. \end{aligned} \tag{3.5}$$

On the other hand, Lemmas 2.2 can be used to establish the estimates

$$\begin{aligned} \|P_{\phi,\mathscr{A}}\boldsymbol{\phi} - P_{\psi,\alpha}\boldsymbol{\psi}\|_{(h)} &\leqslant C_1(\|\xi\|_{(h)} + \|\zeta\|_{(h)}), \\ \|Q_\phi\mathscr{A} - Q_\psi\boldsymbol{\alpha}\|_{(h)} &\leqslant C_1(\|\xi\|_{(h)} + \|\zeta\|_{(h)}), \\ \|\mathbf{R}_\phi - \mathbf{R}_\psi\|_{(h)} &\leqslant C_1\,\|\xi\|_{(h)}, \end{aligned} \tag{3.6}$$

with C_1 depending only on K, K', and $\sup_{t\geqslant 0}|H(t)|$.

Using (3.4)–(3.6), the fact that $S\geqslant 0$, and the Gronwall inequality, we immediately reach the following error control in the integral norm:

$$\|\xi(t)\|^2_{(h)} + \|\zeta(t)\|^2_{(h)} \leqslant C_2 T h^4 e^{C_3 T}, \qquad 0\leqslant t\leqslant T, \tag{3.7}$$

where $C_2, C_3 > 0$ depend on C, C_1.

To get the expected pointwise error estimate, we need to find suitable bounds for $(\xi, S\xi)_{(h)}$ and $(\zeta, S\zeta)_{(h)}$.

From (3.4)–(3.7) and a simple interpolation inequality, it follows that

$$\begin{aligned} &\frac{1}{2}\frac{d}{dt}((\xi, S\xi)_{(h)} + (\zeta, S\zeta)_{(h)}) \\ &\quad\leqslant -\|S\xi\|^2_{(h)} - \|S\zeta\|^2_{(h)} + (\|P_{\phi,\mathscr{A}}\boldsymbol{\phi} - P_{\psi,\alpha}\boldsymbol{\psi}\|_{(h)} + \|\boldsymbol{\eta}_1\|_{(h)})\,\|S\xi\|_{(h)} \\ &\qquad + (\|Q_\phi\mathscr{A} - Q_\psi\boldsymbol{\alpha}\|_{(h)} + \|\mathbf{R}_\phi - \mathbf{R}_\psi\|_{(h)} + \|\boldsymbol{\eta}_2\|_{(h)})\,\|S\zeta\|_{(h)} \\ &\quad\leqslant C_4 h^4 e^{C_5 T}, \qquad 0\leqslant t\leqslant T \end{aligned}$$

with $C_4, C_5 > 0$ depending only on C, C_2, C_3, which implies the bound

$$(\xi, S\xi)_{(h)}(t) + (\zeta, S\zeta)_{(h)}(t) \leqslant T C_4 h^4 e^{C_5 T}, \qquad 0\leqslant t\leqslant T. \tag{3.8}$$

Finally, combining (3.2), (3.7), and (3.8), one achieves the following pointwise error control

$$\sup_{1\leqslant i\leqslant M,\, 0\leqslant t\leqslant T} \max\{|\xi_i(t)|, |\zeta_i(t)|\} \leqslant T C_6 h^2 e^{C_7 T},$$

where $C_6, C_7 > 0$ are determined by l and C_j $(j = 2, ..., 5)$.

The proof of Theorem 2.1 is complete.

Now the semi-discretized system (2.3) may further be discretized in the time variable by various finite difference schemes. For our purpose, we choose to use the backward or implicit difference scheme to discretize the time. In this manner, although (2.3) is nonlinear, a maximum principle argument enables us to prove the stability of the scheme in the pointwise norm and, then, the convergence will follow readily. Such an analysis is presented in the next section. A series of numerical results obtained by this scheme and their interesting physical implications will be detailed in Section 5.

4. Analysis of the Backward Difference Scheme

On a given finite time interval $[0, T]$, $T > 0$, let $k = T/N$ (where $N > 0$ is an integer) be the discretized time step and

$$t_j = jk, \qquad j = 0, 1, ..., N$$

the mesh points. With the notation

$$\phi_i^j = \phi(x_i, t_j), \qquad \mathscr{A}_i^j = \mathscr{A}(x_i, t_j), \qquad i = 1, ..., M, \qquad j = 0, 1, ..., N,$$
$$\Delta^2 u_i = u_{i+1} - 2u_i + u_{i-1}, \qquad i = 1, ..., M,$$

and after replacing ϕ_t and $\mathscr{A}_t$ at $x = x_i, t = t_{j+1}$ by $(\phi_i^{j+1} - \phi_i^j)/k$ and $(\mathscr{A}_i^{j+1} - \mathscr{A}_i^j)/k$, we can rewrite (2.1) as

$$\begin{aligned} \phi_i^{j+1} &= \phi_i^j + r\,\Delta^2\phi_i^{j+1} - \lambda k([\phi_i^{j+1}]^2 \\ &\quad -1 + H^2(t_{j+1})[\mathscr{A}_i^{j+1} + x_i]^2)\,\phi_i^{j+1} + \mu_i^{j+1}, \\ \mathscr{A}_i^{j+1} &= \mathscr{A}_i^j + r\,\Delta^2\mathscr{A}_i^{j+1} - k(\phi_i^{j+1})^2\,(\mathscr{A}_i^{j+1} + x_i) + v_i^{j+1}, \\ &\quad j = 0, 1, ..., N-1; \\ \phi_i^0 &= \phi_0(x_i), \qquad \mathscr{A}_i^0 = \mathscr{A}_0(x_i), \end{aligned} \tag{4.1}$$

where $r = k/h^2$, $\phi_0^j = \phi_1^j$, $\phi_M^j = \phi_{M+1}^j$, $\mathscr{A}_0^j = \mathscr{A}_1^j$, $\mathscr{A}_M^j = \mathscr{A}_{M+1}^j$, $i = 1, ..., M$, and μ_i^j, v_i^j satisfy

$$\begin{aligned} kE_T \equiv \max_{i,j}\{|\mu_i^j|, |v_i^j|\} &\leqslant C(k^2 + kh^2) \\ &\quad \times \sup_{-l \leqslant x \leqslant l,\, 0 \leqslant t \leqslant T} \{|\phi_{tt}|, |\mathscr{A}_{tt}|, |D^4\phi|, |D^4\mathscr{A}|\}. \end{aligned}$$

Therefore, neglecting the error terms μ_i^j, v_i^j, and replacing ϕ_i^j, $\mathscr{A}_i^j$ by ψ_i^j, α_i^j in (4.1), we have the following implicit scheme

$$\begin{aligned} \psi_i^{j+1} &= \psi_i^j + r\,\Delta^2\psi_i^{j+1} - \lambda k([\psi_i^{j+1}]^2 \\ &\quad -1 + H^2(t_{j+1})[\alpha_i^{j+1} + x_i]^2)\,\psi_i^{j+1}, \\ \alpha_i^{j+1} &= \alpha_i^j + r\,\Delta^2\alpha_i^{j+1} - k(\psi_i^{j+1})^2\,(\alpha_i^{j+1} + x_i), \\ &\quad j = 0, 1, ..., N-1; \\ \psi_i^0 &= \phi_0(x_i), \qquad \alpha_i^0 = \mathscr{A}_0(x_i), \end{aligned} \tag{4.2}$$

with the boundary condition $\psi_0^j = \psi_1^j$, $\psi_M^j = \psi_{M+1}^j$, $\alpha_0^j = \alpha_1^j$, $\alpha_M^j = \alpha_{M+1}^j$.

The following lemma concerning the stability of the backward scheme (4.2) is easily proved by a maximum principle argument.

LEMMA 4.1. *With the notation* $K=\max\{1, |\phi_0|_0\}$ *and* $K'=\max\{l, |\mathscr{A}_0|_0\}$ *(see Lemma 2.2), we have* $|\psi_i^j| \leqslant K$ *and* $|\alpha_i^j| \leqslant K'$.

Proof. Suppose otherwise there were $i_0: 1 \leqslant i_0 \leqslant M$ and $j_0: 1 \leqslant j_0 \leqslant N$ such that

$$\psi_{i_0}^{j_0} = \sup_{i,j} \psi_i^j > K.$$

Then the structure of Eq. (4.2) would lead to a contradiction under the substitution $j+1=j_0$, $i=i_0$. Hence $\psi_i^j \leqslant K$. Similarly one shows $\psi_i^j \geqslant -K$.

We now verify the bound for $|\alpha_i^j|$. Suppose $\sup \alpha_i^j > K'$. Let $j_0: 1 \leqslant j_0 \leqslant N$ satisfy

$$j_0 = \min\{j'=1, ..., N \mid \alpha_{i_0}^{j'} = \max_{i,j} \alpha_i^j\}.$$

Inserting $j_0 = j+1$, $i=i_0$ into (4.2) we find $(\psi_{i_0}^{j_0})^2 (\alpha_{i_0}^{j_0} + x_{i_0}) < 0$. This violates our assumption. By the same way, we can prove $\inf \alpha_i^j \geqslant -K'$. So the lemma follows.

From Eqs. (4.1) and (4.2), the governing equations for the errors $\xi_i^j = \phi_i^j - \psi_i^j$, $\zeta_i^j = \mathscr{A}_i^j - \alpha_i^j$ are

$$\begin{aligned} &r\,\Delta^2 \xi_i^{j+1} - \xi_i^{j+1} = f_i^{j+1}, \\ &r\,\Delta^2 \zeta_i^{j+1} - \zeta_i^{j+1} = g_i^{j+1}, \\ &\xi_i^0 = 0, \qquad \zeta_i^0 = 0, \end{aligned} \tag{4.3}$$

where

$$\begin{aligned} f_i^{j+1} = &-\xi_i^j + \lambda k([\phi_i^{j+1}]^2 - 1 + H^2(t_{j+1})[\mathscr{A}_i^{j+1} + x_i]^2)\,\phi_i^{j+1} \\ &- \lambda k([\psi_i^{j+1}]^2 - 1 + H^2(t_{j+1})[\alpha_i^{j+1} + x_i]^2)\,\psi_i^{j+1} - \mu_i^{j+1}, \\ g_i^{j+1} = &-\zeta_i^j + k(\phi_i^j)^2\,(\mathscr{A}_i^{j+1} + x_i) - k(\psi_i^j)^2\,(\alpha_i^{j+1} + x_i) - \nu_i^{j+1}. \end{aligned}$$

Using the boundary condition $\xi_0^j = \xi_1^j$, $\xi_M^j = \xi_{M+1}^j$, $\zeta_0^j = \zeta_1^j$, $\zeta_M^j = \zeta_{M+1}^j$, and a maximum principle argument in (4.3) as in [8], we find

$$\max_i |\xi_i^{j+1}| \leqslant \max_i |f_i^{j+1}|, \qquad \max_i |\zeta_i^{j+1}| \leqslant \max_i |g_i^{j+1}|. \tag{4.4}$$

Therefore, it follows from Lemma 4.1 and (4.4) that

$$\begin{aligned} \max_i |\xi_i^{j+1}| \leqslant{}& \max_i |\xi_i^j| + \lambda k(3K^2 + \sup_t H^2(t)(K'^2 + 2lK' + l^2) + 1) \max_i |\xi_i^{j+1}| \\ &+ 2\lambda k K \sup_t H^2(t)(K' + l) \max_i |\zeta_i^{j+1}| + \max_i |\mu_i^{j+1}|, \\ \max_i |\zeta_i^{j+1}| \leqslant{}& \max_i |\zeta_i^j| + 2kK(K' + l) \max_i |\xi_i^{j+1}| + kK^2 \max_i |\zeta_i^{j+1}| + \max_i |\nu_i^{j+1}|. \end{aligned}$$

Define

$$\theta = \max\{\lambda(3K + \sup_t H^2(t)(K'^2 + 2lK' + l^2) + 1) + 2K(K' + l), 2\lambda K \sup_t H^2(t)(K' + l) + K^2\}. \tag{4.5}$$

Given $\varepsilon \in (0, 1)$, let k be sufficiently small so that $k\theta \leqslant 1 - \varepsilon$. Consequently, the initial condition $\xi_i^0 = 0$, $\zeta_i^0 = 0$ implies the inequality

$$\max_i |\xi_i^{j+1}| + \max_i |\zeta_i^{j+1}| \leqslant (1 - k\theta)^{-1} (\max_i |\xi_i^j| + \max_i |\zeta_i^j|) + 2k(1 - k\theta)^{-1} E_T$$
$$\leqslant 2E_T T(1 - \theta T/N)^{-N} \leqslant 2E_T T\varepsilon^{-\theta T/(1-\varepsilon)}.$$

It may be verified by Lemma 3.1, Eqs. (2.1), and the embedding

$$H^k(-l, l) \to C^{k-1}[-l, l]$$

that the conditions $\phi_0, \mathscr{A}_0 \in H^5(-l, l)$ and $\sup_t(|H(t)| + |\dot{H}(t)|) < \infty$ ensure that the quantity

$$\sup_{-l \leqslant x \leqslant l, t \geqslant 0} \max\{|\phi_{tt}(x, t)|, |\mathscr{A}_{tt}(x, t)|, |D^4\phi(x, t)|, |D^4\mathscr{A}(x, t)|\}$$

can be bounded by a constant depending only on l, λ, $\|\phi_0\|_5$, $\|\mathscr{A}_0\|_5$, and $\sup_t(|H(t)| + |\dot{H}(t)|)$. Hence, we have proved

THEOREM 4.2. *Suppose* $(\phi(x, t), \mathscr{A}(x, t))$ *is the solution of Eqs.* (2.1) *where* $\phi_0, \mathscr{A}_0 \in H^5(-l, l)$ *and* $H(t)$ *is a* C^1 *function so that* $\sup_{t \geqslant 0}(|H(t)| + |\dot{H}(t)|) < \infty$ *and* $\{(\psi_i^j, \alpha_i^j)\}$ *the sequence determined by the backward scheme* (4.2). *Let* θ *be as defined in* (4.5). *For any* $\varepsilon \in (0, 1)$, *we have the error estimate*

$$\max\{|\phi(x_i, t_j) - \psi_i^j|, |\mathscr{A}(x_i, t_j) - \alpha_i^j|\} \leqslant \delta(k + h^2)\, T\varepsilon^{-\theta T/(1-\varepsilon)},$$

where $k\theta \leqslant 1 - \varepsilon$ *or* $N \geqslant \theta T/(1 - \varepsilon)$ *and* $\delta > 0$ *is a constant depending only on* l, λ, $\|\phi_0\|_5$, $\|\mathscr{A}_0\|_5$, *and* $\sup_{t \geqslant 0}(|H(t)| + |\dot{H}(t)|)$.

Note. Since our purpose is to calculate the physical states of a superconducting film under the influence of an external source $H = H_0 \neq 0$ by connecting these states with the states at $H = 0$, so ϕ_0 and $\mathscr{A}_0$ are determined by (1.2):

$$\phi_0 = \pm 1, \qquad \mathscr{A}_0 = \sinh x/\cosh l - x.$$

Therefore $K = 1$, $K' = \max\{1, l\}$, and constant θ is easily evaluated.

5. Numerical Results

In this section we present a series of numerical results obtained by the gradient flow method analyzed in the previous sections. Although, in principle, the physical solutions of Eqs. (1.1) are to be found in the $t \to \infty$ limit of the solutions of Eqs. (1.4) where ϕ_0, A_0 satisfy (1.2), our computations carried out up to a large value of the coupling constant $\lambda = 1000$ show that the actual convergence time is quite short. In all of the examples here, the approximations are already impressively satisfactory after a run with $T = 5$–164. This suggests that our method may provide an efficient and practical tool for computing various aspects of thin film superconductivity.

Recall that, the normal and superconducting states are characterized respectively by solutions of Eqs. (1.1) satisfying $\phi(x) \equiv 0$, $A'(x) \equiv 1$ and $\phi(x) \not\equiv 0$, $A'(x) \not\equiv 1$. In our experiments below we are interested in the phase transitions from normal to superconducting states, and vice versa, as one varies the external magnetic field H and the coupling constant λ. A sufficient condition has been established earlier [20] which ensures the occurrence of the superconducting phase. This condition reads

$$l^2 H^2 \leqslant \tfrac{3}{2}. \tag{5.1}$$

Occasionally, we will use this condition as a reference for choosing the strength of the external field.

The numerical scheme used in this section is the backward finite difference method analyzed in Section 4. Let us first explain briefly the computational procedure taken here.

With the notation of Section 4, put

$$U^j = (\psi_1^j, ..., \psi_M^j, \alpha_1^j, ..., \alpha_M^j), \qquad j = 0, 1, ..., N.$$

We may write Eqs. (4.2) as

$$\mathscr{L}(U^{j+1}) = U^j + \Gamma(U^{j+1}), \tag{5.2}$$

where

$$\mathscr{L}(U^j) = (\psi_1^j - r\,\Delta^2\psi_1^j, ..., \psi_M^j - r\,\Delta^2\psi_M^j, \alpha_1^j - r\,\Delta^2\alpha_1^j, ..., \alpha_M^j - r\,\Delta^2\alpha_M^j),$$

and the form of $\Gamma(U^j)$ is self-evident. Knowing U^j, we must determine U^{j+1}. Since (5.2) is an implicit equation, an iterative method has to be introduced. The iterative sequence $\{U^{j+1,m}\}_{m=0}^{\infty}$ is defined as follows.

$$U^{j+1,0} = U^j,$$

$$\mathscr{L}(U^{j+1,m+1}) = U^j + (f(U^{j+1,m+1}, U^{j+1,m}), g(U^{j+1,m+1}, U^{j+1,m})),$$

with

$$f(U^{j+1,m+1}, U^{j+1,m})$$
$$= -\lambda k(H^2(t_{j+1})[\alpha_i^{j+1,m} + x_i]^2 \psi_i^{j+1,m+1} + [(\psi_i^{j+1,m})^2 - 1]\, \psi_i^{j+1,m})_{i=1}^M,$$

$$g(U^{j+1,m+1}, U^{j+1,m})$$
$$= -k([\psi_i^{j+1,m}]^2 \alpha_i^{j+1,m+1} + [\psi_i^{j+1,m}]^2 x_i)_{i=1}^M.$$

The iteration terminates when

$$|U^{j+1,m+1} - U^{j+1,m}| \equiv \sup_i |\psi_i^{j+1,m+1} - \psi_i^{j+1,m}| + \sup_i |\alpha_i^{j+1,m+1} - \alpha_i^{j+1,m}| < 10^{-7} \tag{5.3}$$

and $\Gamma(U^{j+1})$ is then approximated by $(f(U^{j+1,m+1}, U^{j+1,m}),\ g(U^{j+1,m+1}, U^{j+1,m}))$. In all of our experiments, the accuracy (5.3) can be reached after 5–10 steps. This completes one step in the implicit iterative scheme (5.2).

For the scheme (5.2), our calculation terminates if the accuracy

$$|U^{j+1} - U^j| < 10^{-8}$$

is achieved, which means that a steady state solution is found: the discretized gradient flow $\{U^j\}$ converges to a physical state of the superconducting film. Obviously, in different parameter regions, the required time for the computation varies greatly.

For convenience, in what follows, we will fix $l = 1$ unless otherwise stated.

EXAMPLE 5.1. We first examine that the numerical solutions of Eqs. (1.1) at $H = H_0$ obtained by connecting the states at $H = 0$ through the gradient flow (1.3) are independent of the choice of the "connecting function" $H(t)$: $H(0) = 0$, $H(t) = H_0$, $t \geqslant$ some $t_0 > 0$.

For definiteness, let us set $\lambda = 0.3$ (type I superconductivity), $M = 101$, and $r = 50$ in the scheme (4.2) or (5.2). If $H_0 = 2$, (5.1) is violated and we may expect to find a normal state solution. Two connecting functions are taken:

$$F(t) = \min\{t, H_0\}, \qquad G(t) = \min\{0.5t + \sin 2\pi t, H_0\}. \tag{5.4}$$

$F(t) \equiv H_0$ after $t \geqslant 2$ and is strictly monotone in $[0, 2)$ but $G(t) \equiv H_0$ for $t \geqslant 6$ and oscillates in $[0, 6)$. For both cases, the numerical solutions converge to the normal state $\phi = 0$, $A = x$ (the computation terminates at $t = 164$).

Figure 5.1a illustrates the energy decay corresponding to different connecting functions. Initially, the two curves differ greatly, but they soon approach the lowest energy level $E = 0.15$.

Figure 5.1b displays the behaviour of the excited magnetic field $B(x, t) = H(t)\,DA(x, t)$ with $H(t) = F(t)$. As time t increases from $t = 0.48$ to 164, the transition from superconducting states to the normal state develops. Eventually, the external field completely penetrates the film and superconductivity is quenched. The curves from the bottom to the top are ordered by increasing time.

EXAMPLE 5.2. Let the data λ, M, r be the same as in Example 5.1. Choose $H = H_0 = 1$ and the connecting function $H(t) = F(t)$ (cf. (5.4)). From (5.1) we know that the film is in the superconducting phase. In our computation, the energy

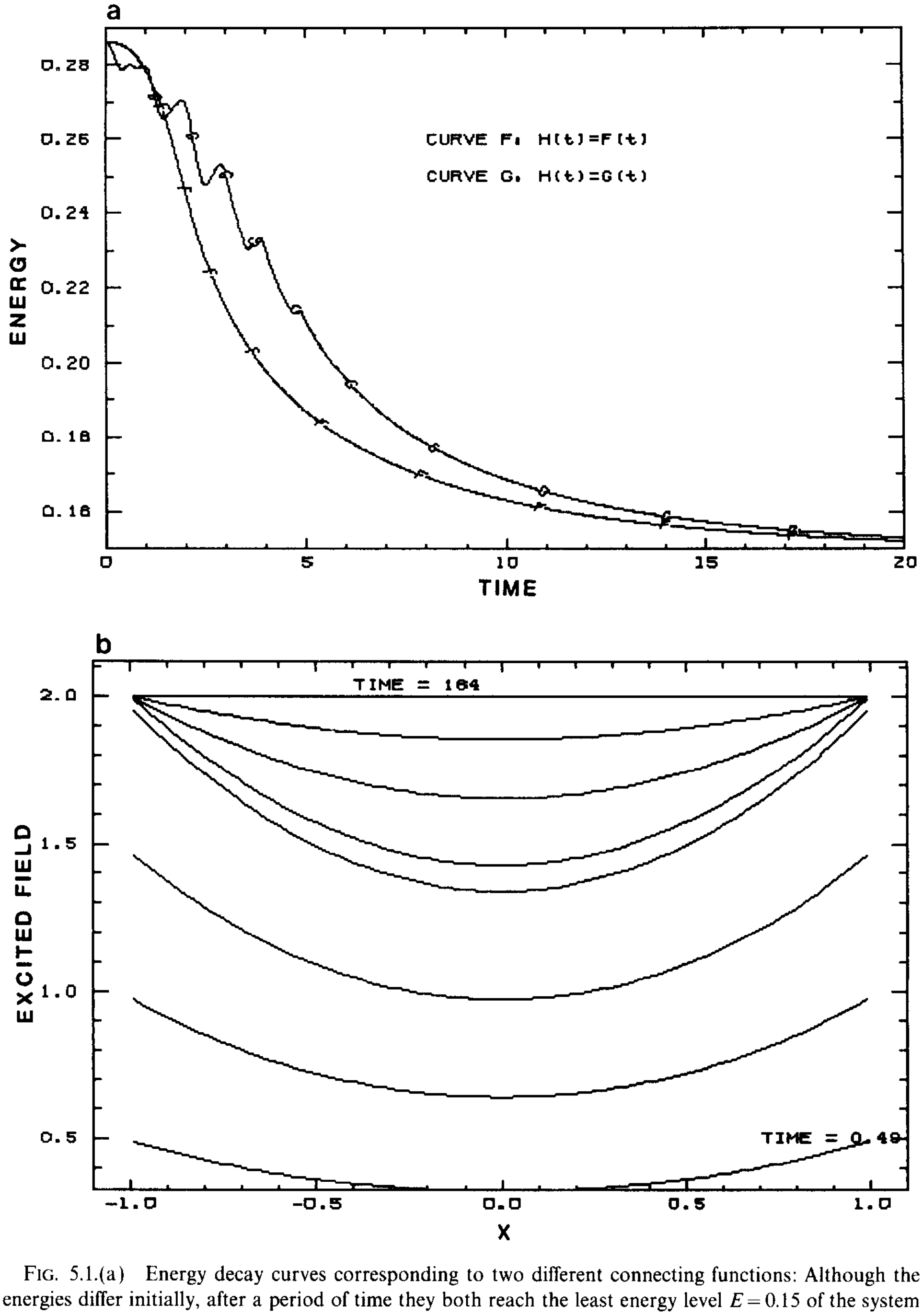

FIG. 5.1.(a) Energy decay curves corresponding to two different connecting functions: Although the energies differ initially, after a period of time they both reach the least energy level $E=0.15$ of the system at $H=2$ and the sample then stays in the normal phase. Thus, the evolution history is not important in the Ginzburg-Landau theory. (b) Development of the state from the completely superconducting phase to the normal phase: Eventually no superconducting electron pairs can survive and the sample is penetrated by the external field like a normal conductor.

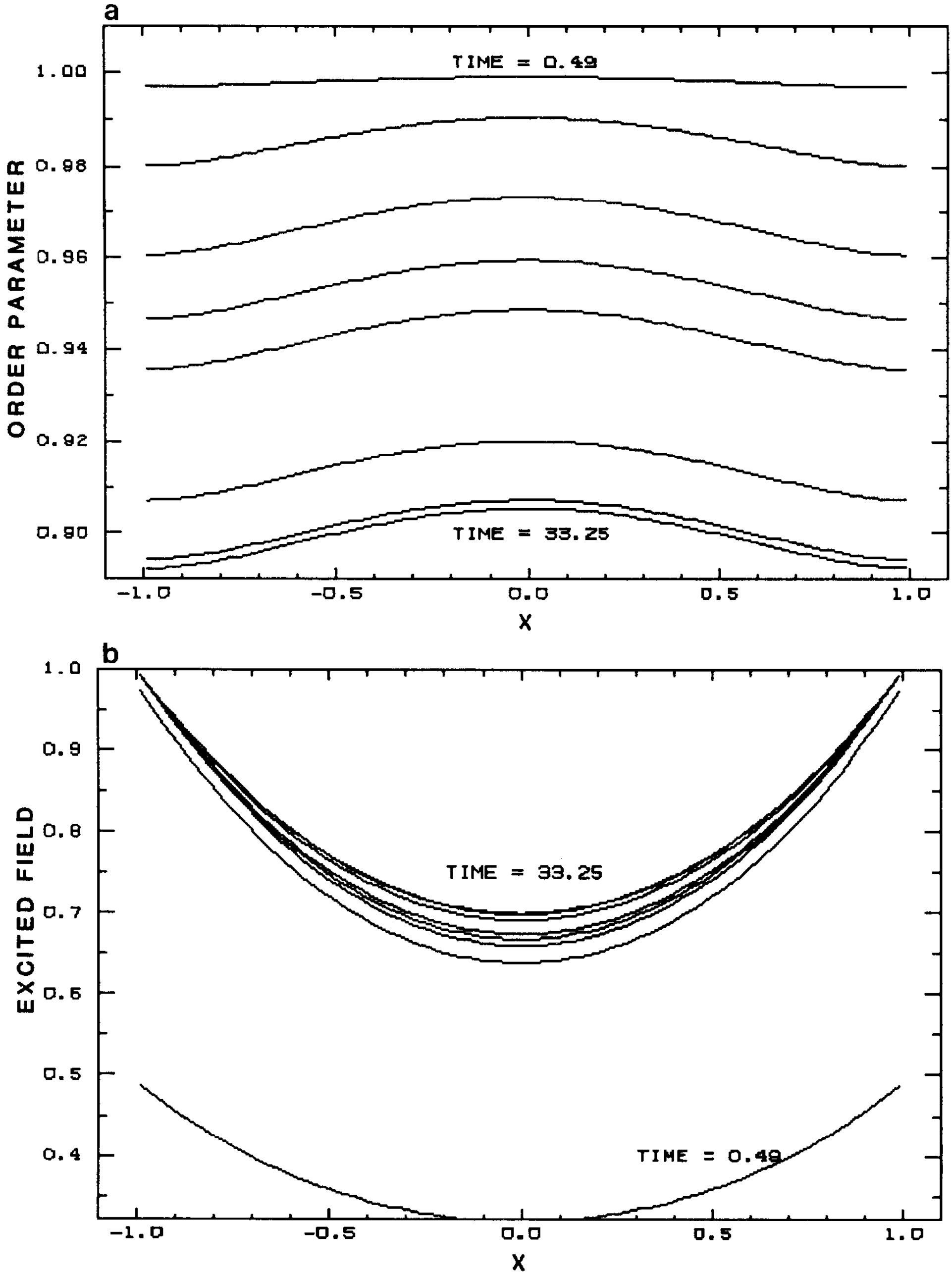

FIG. 5.2.(a) Behaviour of the order parameter ϕ at different time stages: In the large time limit the flow approaches a least energy solution of the system and the sample is in a superconducting state so that a symmetric nucleation of superconductivity is maintained. The strength of the external field is neither weak enough to leave the film in the completely superconducting states nor sufficiently strong to destroy superconductivity. (b) Partial penetration of the external field: The regions near the surfaces of the film are almost in the normal state due to the influence of a sufficiently strong external source and the penetration strength attains its minimum at the center of the sample.

decays after a short period of time and the numerical solutions converge to a superconducting state (the program halts at $t = 33.25$).

Figure 5.2a shows the behaviour of the order parameter ϕ at different time stages. The curves from the top to the bottom are ordered by increasing time $t = 0.49$–33.25. At $t = 0.49$, since the external field is still weak, the film is almost in the completely superconducting state and the density of the Cooper pairs stays close to its maximum value $\phi = 1$. As time develops and the external field becomes strong, the superconducting electron pairs can hardly survive near the boundary of the film and they tend to gain a greater density in the middle of the sample. This is known as the nucleation of superconductivity at intermediate external fields.

In Fig. 5.2b, the graphs of the excited field versus the spatial variable x are ordered from the bottom to the top by increasing time $t = 0.49$–33.25. At low field, namely, $t = 0.49$, the external field may only achieve a partial penetration near the surfaces and it is completely screened in the middle of the film. As time develops, the external source becomes strong and the solution steadily approaches a stable state. This state represents a superconducting phase. There is a complete penetration of the external field near the surfaces and the excited field rapidly decays to its minimum at the center of the sample. The magnetic screening is partial.

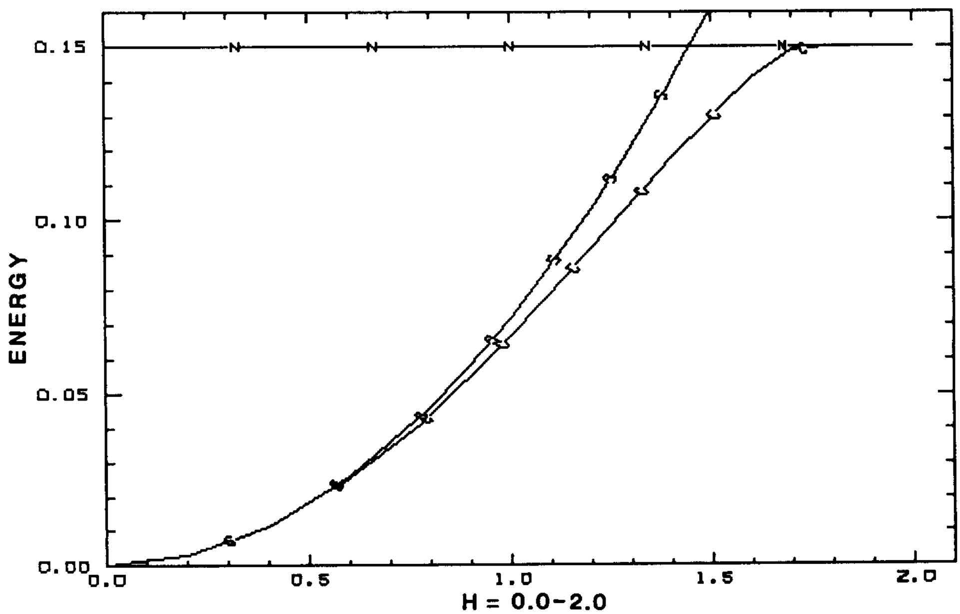

FIG. 5.3. Three branches of energy curves versus the values of the external magnetic field: Letters C, N, S denote the energy curves of the computed solutions, the normal state, and the completely superconducting states (given by (1.2)), respectively. Physical experiments say that the C curve should simply coincides with the S curve (at low fields) and with the N curve (at high fields) since $\lambda = 0.3$ corresponds to type I superconductivity. Our results here show that there is a slight deviation of the Ginzburg-Landau theory from experimental facts at intermediate fields.

EXAMPLE 5.3. Figure 5.3 is the energy curves versus the values of the external magnetic field H of the computed solutions of (1.1), the normal state, and the completely superconducting states given by (1.2). Here $\lambda = 0.3$. These curves are denoted by the letters C, N, and S, respectively. It is seen that the energy of the least energy solutions (the C curve) of Eqs. (1.1) is below the normal state energy level $E = 0.15$ (the N curve) if $H < 1.75$. Therefore the sample is in the superconducting phase. While, for $H > 1.75$, the C curve joins the N curve and the sample is in the normal phase. When $H < 0.6$, the C curve coincides with the S curve and the film is in a completely superconducting state. In the range $0.6 < H < 1.75$, the C curve is strictly below the N and S curves and the sample is in a superconducting state different from those given by (1.2). The magnetic screening is partial even at the center of the film and a symmetric nucleation of superconductivity occurs. These global energy curves provide a very clear picture of phase transitions in terms of changes of the external field and completely verify the Meissner effect.

EXAMPLE 5.4. As a comparison, we remark that the energy curves versus external fields are qualitatively different for type II superconductors. Let us choose the data $\lambda = 10$, $M = 101$, $r = 50$. The computer results are summarized in Fig. 5.4. As in the above example, there are two critical fields, $H_{c_1} = 0.5$ and $H_{c_2} = 3$. For

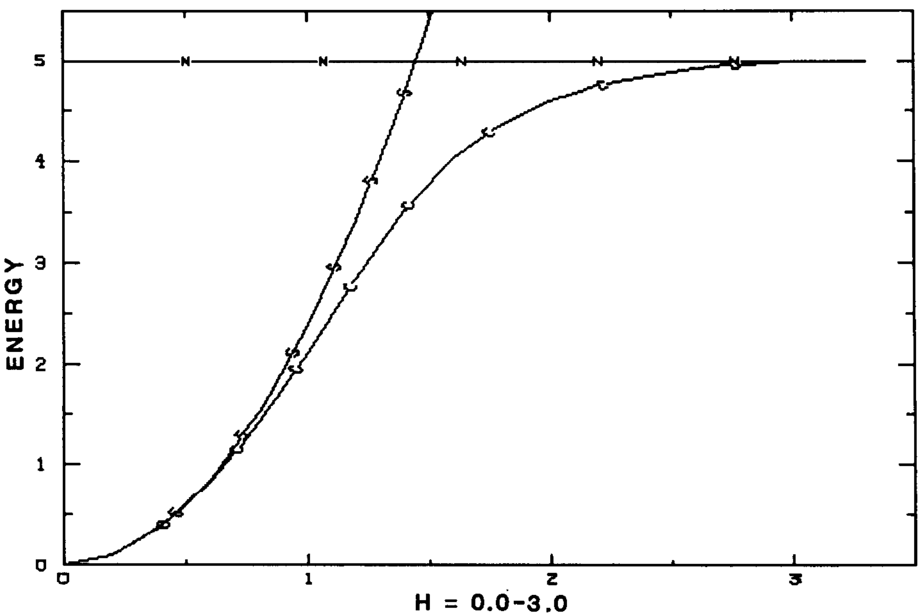

FIG. 5.4. Energy curves versus external fields in type II superconductors: The magnetic behaviour of the sample is now characterized by two critical fields $H_{c_1} = 0.5$ and $H_{c_2} = 3$ which substantially differs from that in type I superconductors. When $H > H_{c_1}$, the realistic energy curve C will bend away from the S curve and finally joint the N curve.

$H < H_{c_1}$, the sample is in a completely superconducting state and behaves like a piece of diamagnetic material. In the range $H_{c_1} < H < H_{c_2}$, the energy curve C of the computed solutions bends away from the curve S and the Abrikosov mixed states [1] are maintained. Finally, when $H > H_{c_2}$, the C curve joins the N curve and the normal phase is reached. This is a characteristic phenomenon of type II superconductivity. It is seen that, in Fig. 5.3 both C and S curves are convex (although there is an inflection point on the C curve near the N curve) and tend to stay close, while, in Fig. 5.4, the C curve is concave after $H = H_{c_1}$ and tends to stay away from the S curve. In fact, Fig. 5.3 indicates a small deviation of the Ginzburg–Landau theory from physically observed facts in type I superconductors but Fig. 5.4 tells us exactly what really happens in type II superconductors.

EXAMPLE 5.5. We are interested also in the behaviour of solutions when the coupling constant λ takes very large values. Results have been obtained with fixed external field $H = H_0 = 5$ and the values of λ varying in the range 10–1000. We still choose $M = 101$. Note that the expression of θ linearly depends on λ if λ is large and that, by Theorem 4.2, we must require $r\lambda$ small in order to achieve convergence of the backward difference scheme (4.2) or (5.2). In our computer experiments, we find that $r\lambda = 500$ seems to be optimal for the problems discussed here. The calcula-

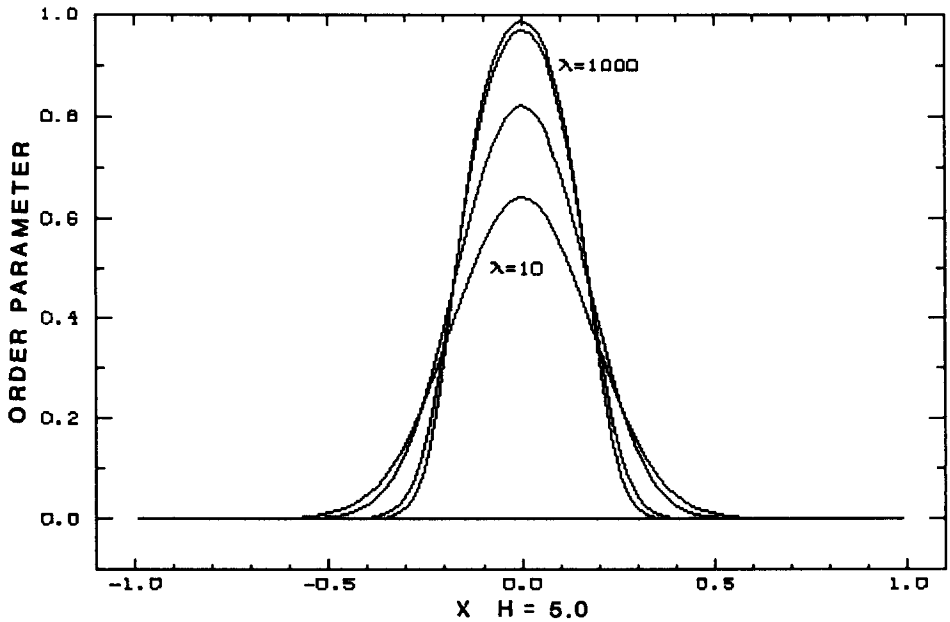

FIG. 5.5. Large λ behaviour of superconducting films: Although the field $H = 5$ is strong enough to quench superconductivity in samples with $\lambda \leqslant 10$, large λ materials can still maintain a superconducting state in regions near the center. In this case superconducting and normal states co-exist. As λ grows, the superconducting core is squeezed into a very narrow region.

tions terminate at $t = 5$–10. The curves of the order parameter ϕ in Fig. 5.5 are ordered from the bottom to the top by increasing values of $\lambda = 10$, 50, 100, 500, 1000. It is seen that, for $\lambda = 10$, the superconducting phase is destroyed and the normal state dominates. The ϕ curve is represented by a horizontal line $\phi = 0$. For larger λ, a superconducting region may be maintained near the center of the sample but finite normal conducting layers also exist. This shows the co-existence of both superconducting and normal regions in a film at intermediate fields in type II superconductivity. As λ increases, the peak of the ϕ curve grows and the density of the Cooper pairs gains a very large value at the center of the sample but the superconducting region is greatly squeezed into a narrow band. This suggests the occurrence of a nonlinear desingularization phenonmenon [1, 3, 4].

Note. The numerical studies in this section have been restricted to a fixed l ($2l$ is the thickness of the film) and treated the external field H as a varying parameter. Similar discussions may be made if one varies l and it can be shown that small or large l favours superconducting states or the normal state as was originally predicted in the celebrated work of Ginzburg and Landau [11].

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